The Dawn of NJOY21 in FY2015

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Introduction

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- Multiple data formats
- Open Source

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- Create a development plan
- Create an ENDF6 reader
- Wrap NJOY2012 for C++

NJOY21 Development Plan

Oversimplified version

- Wrap every Legacy NJOY module in C++
  - C++ is wrapped for Python
- The Legacy modules can be replaced as they are developed in C++

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Several benefits

1. Full functionality from Day 1
2. Preserve familiar interface with Legacy NJOY
3. NJOY21 capabilities will replace Legacy NJOY modules when implemented
4. Command-line option to force use of Legacy NJOY
5. Scripting operation of Legacy NJOY

NJOY21 $\longleftrightarrow$ NJOY2012

Supported modules:

- ACER
- BROADR
- HEATR
- GASPR
- MODER
- PURR
- RECONR
- THERMR
- UNRESR

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- Verification of input parameters
- Errors are caught early
- Faster/easier to diagnose input errors

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- As much automation as possible
- Don't need precise control
- Wrapper must integrate with our build system—`CMake`
- Ability to wrap multiple scripting languages (optional)

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SWIG Widely used, allows for wrapping to multiple target languages

The Dawn of NJOY21

```
commit 0b971051fe7a6cd5ea39b0f10390199dcfc4cd76
Author: Austin Paul McCartney <amccartney@lanl.gov>
Date:   Tue Oct 13 17:52:49 2015 -0600

    First beginning-to-end NJOY21 run completed at 5:43 pm October 13th
```

- New/corrected $S(\alpha, \beta)$ data for SiO_2 processed with NJOY21
- To be made available with next MCNP release

Improving Code Quality

- Several small projects make NJOY21
- Formal expectations for code style and hierarchy.
- Regular code reviews.
- Common build system for all of NJOY21
- Every method is tested
  - $>$90 % test coverage requirement

Conclusion

- NJOY21 Development Plan
- Linking NJOY21 to NJOY2012 Fortran modules
- ENDF6 Parser
- Python wrapping

One More Thing...

http://njoy.github.io/

- Open source license
- No export control
- Encourage contribution and collaboration

Extra Slides

Problematic Input Deck

```
thermr
 43 44 45
 101 1301 8 1 2 1 1 0 222 2
 296.
 .05 .625
stop
```

```
njoy 2012.50  12feb15                                          03/07/16 17:59:25
******************************************************************************

thermr...                                                                 0.0s

***warning***maximum value of beta limits the allowed energy transfer
the sct approx. will be used for transfers larger than  0.633 ev.

***error in calcem***bad temperature for teff2

77
```

NJOY21 output

```
   ##    ##       ##  #######  ##    ##  #######     ##
   ###   ##       ## ##     ##  ##  ##  ##     ##  ####
   ####  ##       ## ##     ##   ####         ##    ##
   ## ## ##       ## ##     ##    ##     #######     ##
   ##  #### ##    ## ##     ##    ##    ##           ##
   ##   ### ##    ## ##     ##    ##    ##           ##
   ##    ##  ######   #######     ##    #########  ######
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

   NJOY21 0.2.0

   Git remote url:
   ssh://git@xcp-stash.lanl.gov:7999/njoy21/njoy21.git

   Git branch:
   development
 ~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~~

2016-03-07 17:58:07,975 INFO  Input parser generated
2016-03-07 17:58:07,975 INFO  Input parsing has started
2016-03-07 17:58:07,976 INFO  Card 1 parsed successfully
2016-03-07 17:58:07,976 ERROR natom argument must be greater than or equal to 1
2016-03-07 17:58:08,003 INFO  Error while parsing card 2
2016-03-07 17:58:08,003 INFO  Error while processing THERMR command
2016-03-07 17:58:08,003 INFO  Error encountered during InputParser parse method
2016-03-07 17:58:08,003 INFO  Error encountered during execution
2016-03-07 17:58:08,003 INFO  NJOY21 will now terminate
```